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Material Damage and Failure

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Abstract

The Material Damage and Failure area seeks to improve and expand fundamental computational and physical knowledge of the material failure process. This is a broad area and it underpins many applications. Substantial ongoing efforts in material failure prediction exist in the NNSA Defense Program Laboratories. The intent of this paper is not to provide a list of ongoing material failure projects in the Laboratories but rather, present a comprehensive description of the pertinent issues in material damage and failure prediction that are currently facing the Laboratories. We particularly seek innovative ideas and collaborations that enhance our capabilities to predict material failure in these topical areas.

Introduction

Predicting the process of material failure and fracture is an extremely challenging scientific problem, central to a number of applications from the performance of munitions to explosive forming processes to predicting the long-time structural integrity of engineered structures. The conditions can range from quasi-static tensile failure to high strain rate shock loading, for example the failure of metals under explosive loading. To predict the component and system performance, safety and reliability under this wide variety of conditions also requires the ability to understand the subsequent response of the damaged material. The development of physics-based models that are capable of describing both the failure process and the subsequent response of materials is thus of great interest.

Truly predictive failure models require understanding the process at all relevant length scales, ranging from the atomistic scale where damage is nucleated, through the continuum, where most large scale systems simulations are performed. What are the critical processes at each length scale? How do we integrate models across length scales? How does damage nucleate and evolve in a material under a variety of loading conditions? How much of the microphysics needs to be accounted for explicitly and what can be glossed over? These are all important questions to be addressed.

For example, the damage and failure process for polycrystalline metals is a sophisticated sequence of physical events occurring at different length scales. It is a stochastic process that is influenced by loading state, microstructure, and boundary conditions. Physical manifestations of a ductile process are generally varying combinations of porosity nucleation and growth, as well as shear localization and banding. Brittle behavior often exhibits plastic deformation in combination with mixed mode crack initiation, growth,

crack percolation and ultimately failure. Generally both ductile and brittle behaviors are of interest. Although lower length scale work is invaluable for the articulation of the physical processes leading to failure, there is still strong practical need to develop continuum level tools capable of predicting the phenomena in question.

The problem can be even more complex since under dynamic loading conditions many materials exhibit solid-solid phase transformations. This transformation in crystallographic structure is also a complex stochastic process that may transition between crystallographic structures which may change the response of the material from ductile to brittle or vice-versa. Some crystallographic structures may be prone to exhibit one type of behavior over another. Still others exhibit transitions between ductile and brittle behaviors depending upon loading and strain rate which may or may not be related to a phase transformation.

Standard mechanical strength models for metallic materials spell out the relationship between stress and the resulting strain during elastic and stable plastic deformation. However at some background strain, metals will transition from uniform or homogeneous deformation to heterogeneous or localized unstable behavior. To be predictive, models must capture the fundamental relationships connecting the independent variables of stress, strain-rate, strain, and temperature to specific bulk material responses such as yield strength, strain-hardening, texture evolution, evolution of global damage, subsequent heterogeneous damage such as strain localization and cracking, and finally material failure. Moreover, for the applications-of-interest, we need to predict those responses accurately for extreme conditions such as at large deformation, high strain-rates, high pressures, and high temperatures. Our materials models must therefore be based on quantifiable physical mechanisms, characterized with inexpensive direct experiments, and validated via comparison with small-scale and integral tests.

Although we use metals to illustrate the technical points, our interest is broad and not limited to this class of materials. The following list of topics, though not exhaustive, provides indication of areas of interest:

- Post-Failure material response and subsequent behavior
- Failure simulation capabilities
- Failure under long-term aging and aggressive environments
- Failure simulation spanning long time scales
- Material failure in micro and nano systems

A brief discussion on what is needed in each topical area is given in the following sections.

Post-Failure material response and subsequent behavior

Conventional practices commonly design systems with a large margin against failure, either at the component or system level. This approach can be unnecessarily conservative and provides little insight into the fundamental physical processes underlying failure or

key potential failure modes. The ability to predict post-failure response of materials can potentially enable more cost-efficient designs by assessing design constraints more accurately and providing a more realistic assessment of risks. In most cases, initiation of material failure does not directly translate into system collapse. Understanding how materials fail and also the subsequent load transferring process will result in an efficient system design by realizing the full potential of material load-bearing capabilities.

Failure simulation capabilities

Despite recent advances in computational sciences and engineering, simulation of fracture and failure of materials remains one of the most challenging material science problems extant. The difficulties arise not only from the need for more fundamental understanding of the underlying physical processes in order to motivate physically-based models to describe material failure, but also in developing numerical methods that can treat the changing geometries associated with the creation of new free surfaces and the excessive bulk deformations. The simulation of the behavior of damaged material puts further demands on the ability to simulate the evolution of the failure process. Numerical algorithms that will alleviate the constraints imposed by discretization and mimic the physical process of strength degradation are needed for predictive material failure simulations.

Failure under long-term aging and aggressive environments

The extension of stockpile life has resulted in increased attention to the response of materials under the combination of aging and aggressive environmental conditions. Material failure models are required that can not only predict damage but also assess the full life-cycle for a material, component or system in order to support lifetime predictions, providing the additional challenge of mixing long- and short-time-scale processes. For example, the phenomena of diffusion, corrosion, and oxidation affect performance in most of the systems (micro and macro) of interest. However, little scientific understanding has been developed on the interactions that occur over these larger time scales, and on the magnitude of their effect as compared with mechanistic behavior observed over much shorter times.

Failure simulation spanning long time scales

Critically important to life-cycle predictions is the extension of simulation technologies to very long time scales. While this is currently possible with meso-scale models and simulations, the models in use at these scales are often ad hoc or empirical in nature, limiting their predictive capability. At the microscale, where many of the interesting physical processes begin, the time scales accessible by simulation are very short and are currently inadequate to this task. Development on this topic would have dramatic impact on our ability to model phenomena such as the behavior of impurities/gases in metallic and ceramic materials, adhesion between metallic and polymer thin films on ceramic substrates used in nano-scale devices, and the material property degradation caused by aging processes of corrosion and oxidation.

Failure of micro and nano systems

Nano- and micro-technologies can present particular challenges for new material failure models. Application of conventional continuum mechanics to nano- and micro-systems has been problematic and little understanding of the failure response of such systems exists. Observed size-dependent material behavior adds more complexity to the problem. Development of failure models that can lead to the prediction of nano- and micro-system performance and reliability is encouraged.

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